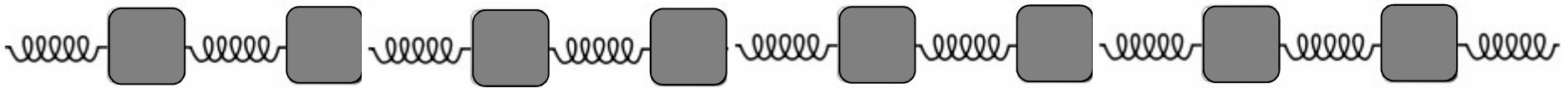
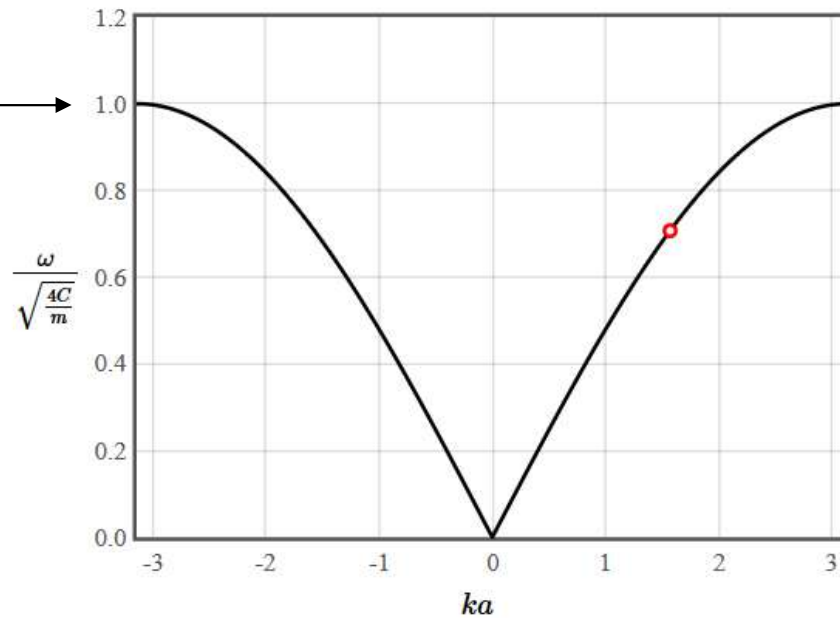


Phonons

Linear Chain - dispersion relation



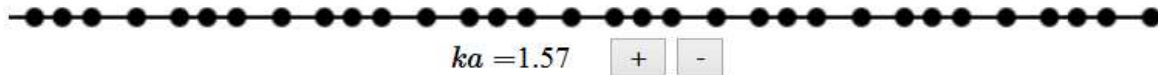
Max. freq. →



$$m \frac{d^2 u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1})$$

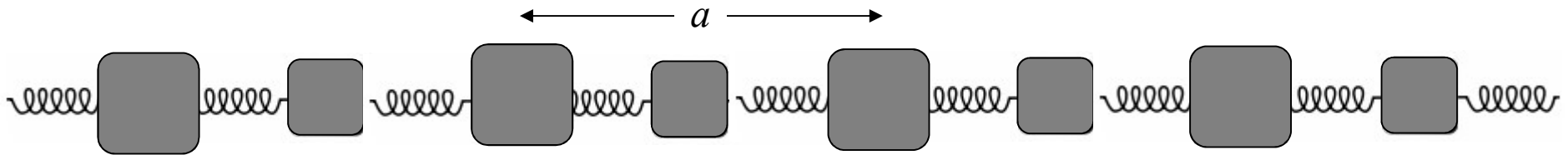
$$u_s = A_k e^{i(ksa - \omega t)}$$

$$\omega = \sqrt{\frac{4C}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|$$



$$\text{speed of sound} = \sqrt{\frac{C}{m}} a$$

Linear chain M_1 and M_2



Newton's law:
$$M_1 \frac{d^2 u_s}{dt^2} = C(v_{s-1} - u_s) + C(v_s - u_s)$$

$2N$ modes
$$M_2 \frac{d^2 v_s}{dt^2} = C(u_s - v_s) + C(u_{s+1} - v_s)$$

assume harmonic
solutions

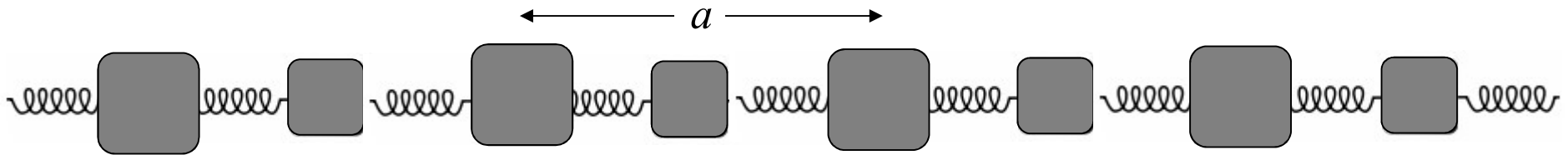
$$u_s = u_k e^{i(ksa - \omega t)}$$

$$v_s = v_k e^{i(ksa - \omega t)}$$

$$-\omega^2 M_1 u_k = C v_k (1 + \exp(-ika)) - 2C u_k$$

$$-\omega^2 M_2 v_k = C u_k (1 + \exp(ika)) - 2C v_k$$

Linear chain M_1 and M_2



$$-\omega^2 M_1 u_k = C v_k (1 + \exp(-ika)) - 2C u_k$$

$$-\omega^2 M_2 v_k = C u_k (1 + \exp(ika)) - 2C v_k$$

$$\begin{bmatrix} \omega^2 M_1 - 2C & C(1 + \exp(-ika)) \\ C(1 + \exp(ika)) & \omega^2 M_2 - 2C \end{bmatrix} \begin{bmatrix} u_k \\ v_k \end{bmatrix} = 0$$

$$M_1 M_2 \omega^4 - 2C(M_1 + M_2) \omega^2 + 2C^2 (1 - \cos(ka)) = 0$$

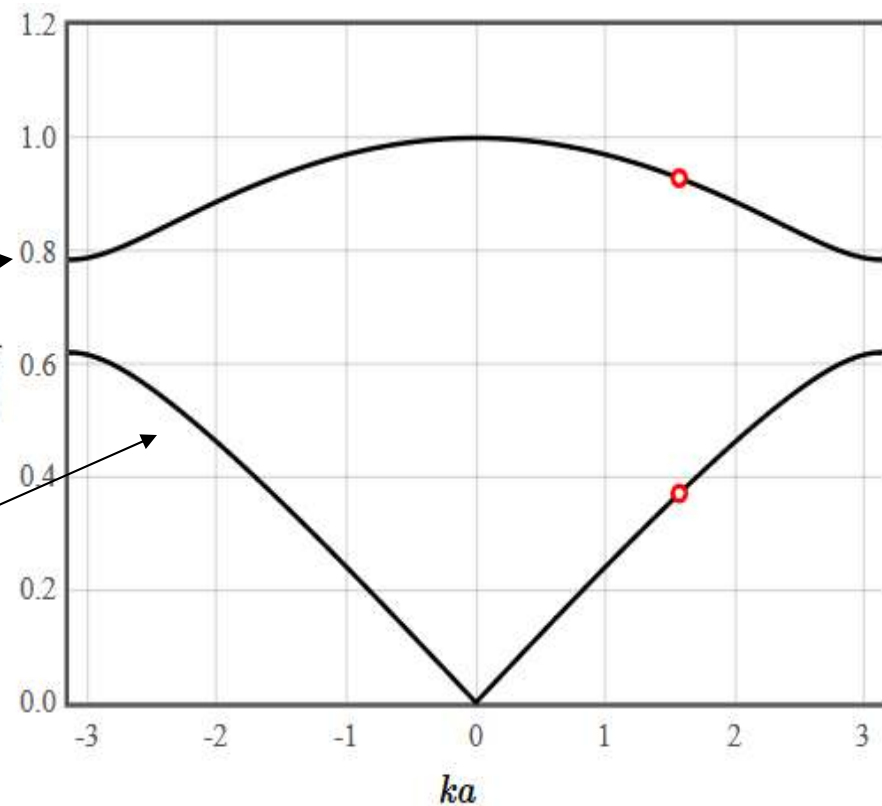
dispersion relation

$$\omega^2 = C \left(\frac{1}{M_1} + \frac{1}{M_2} \right) \pm C \sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4 \sin^2 \left(\frac{ka}{2} \right)}{M_1 M_2}}$$

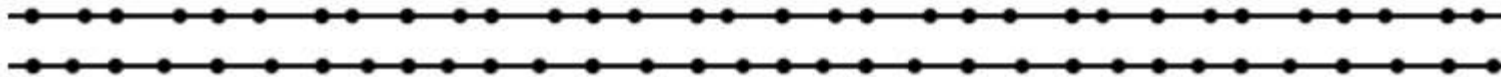
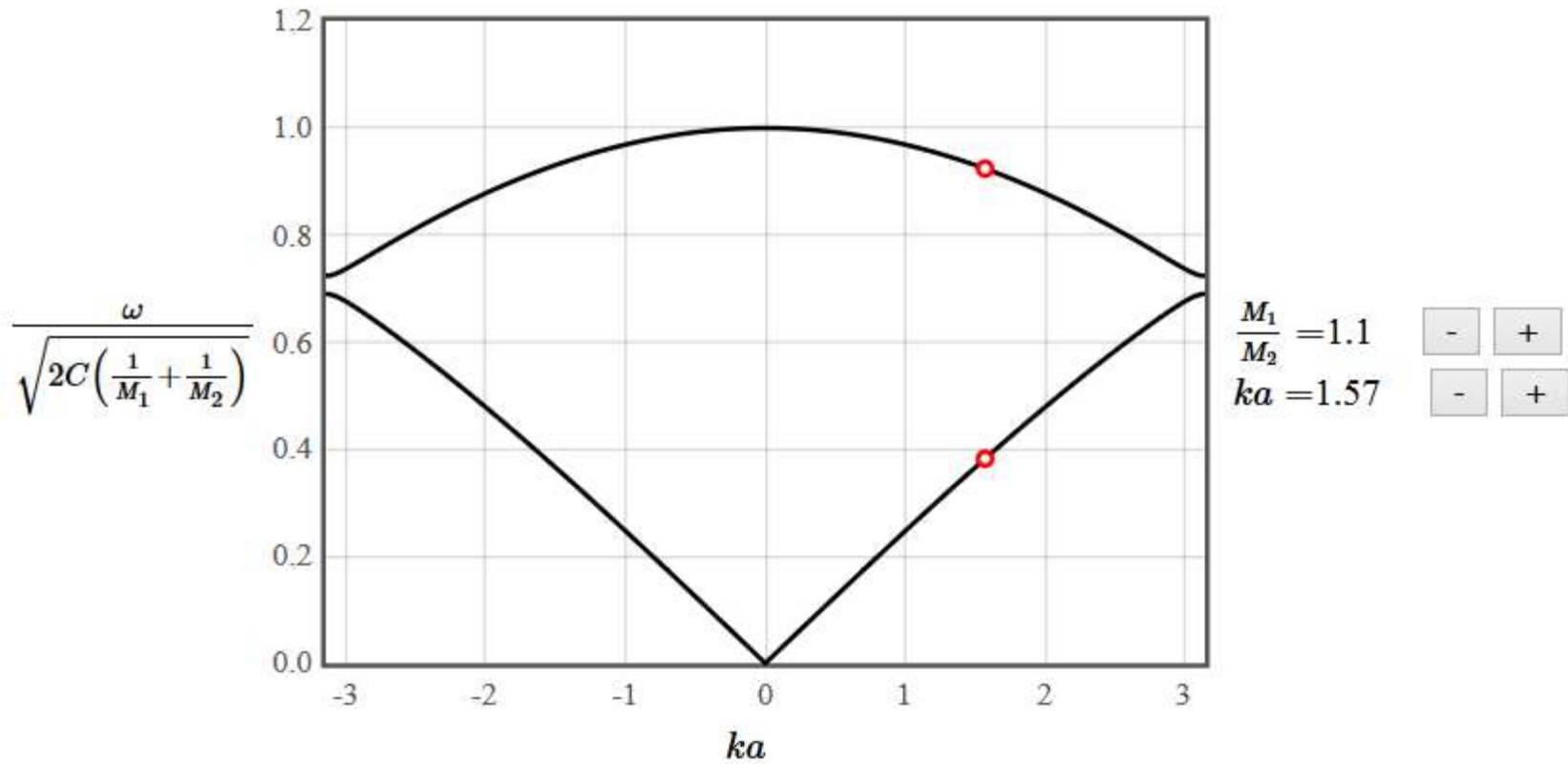
Optical phonon branch

$$\frac{\omega}{\sqrt{2C \left(\frac{1}{M_1} + \frac{1}{M_2} \right)}}$$

Acoustic phonon branch

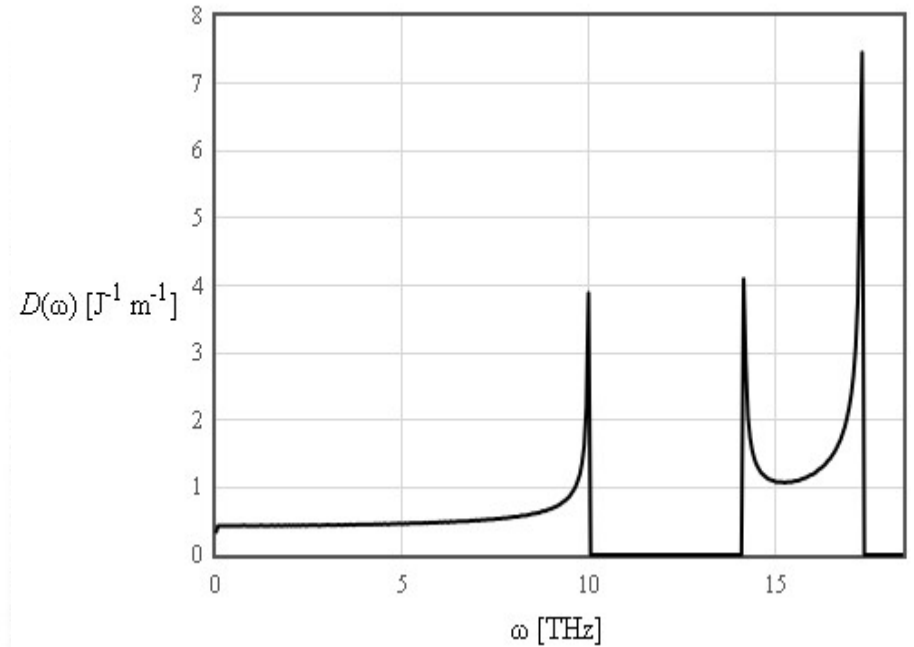
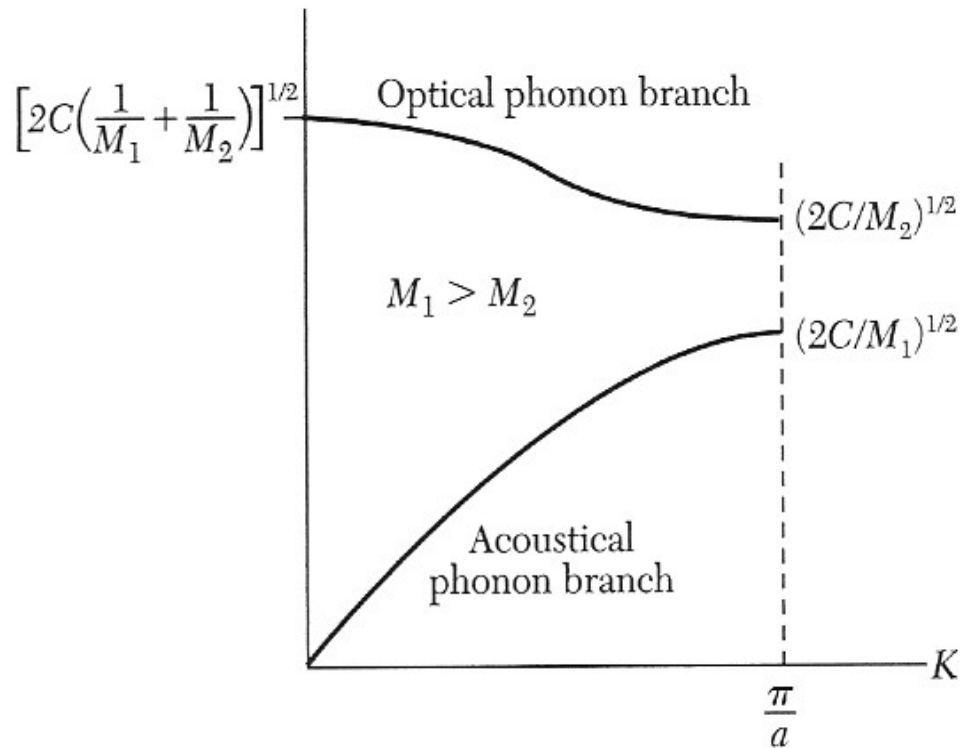


normal modes



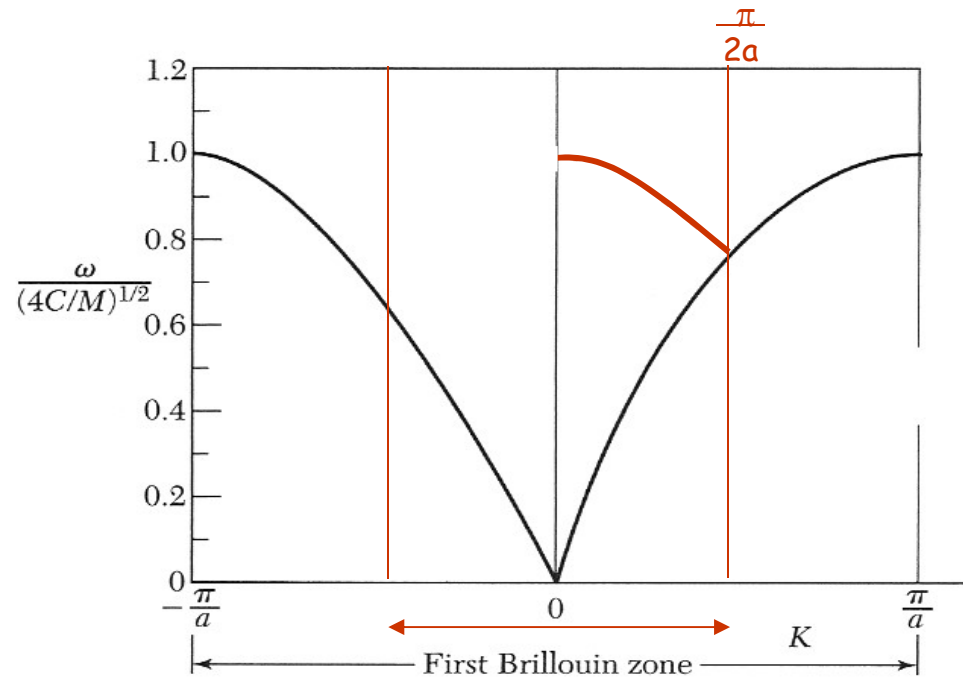
<http://lampx.tugraz.at/~hadley/ss1/phonons/1d/1d2m.php>

density of states

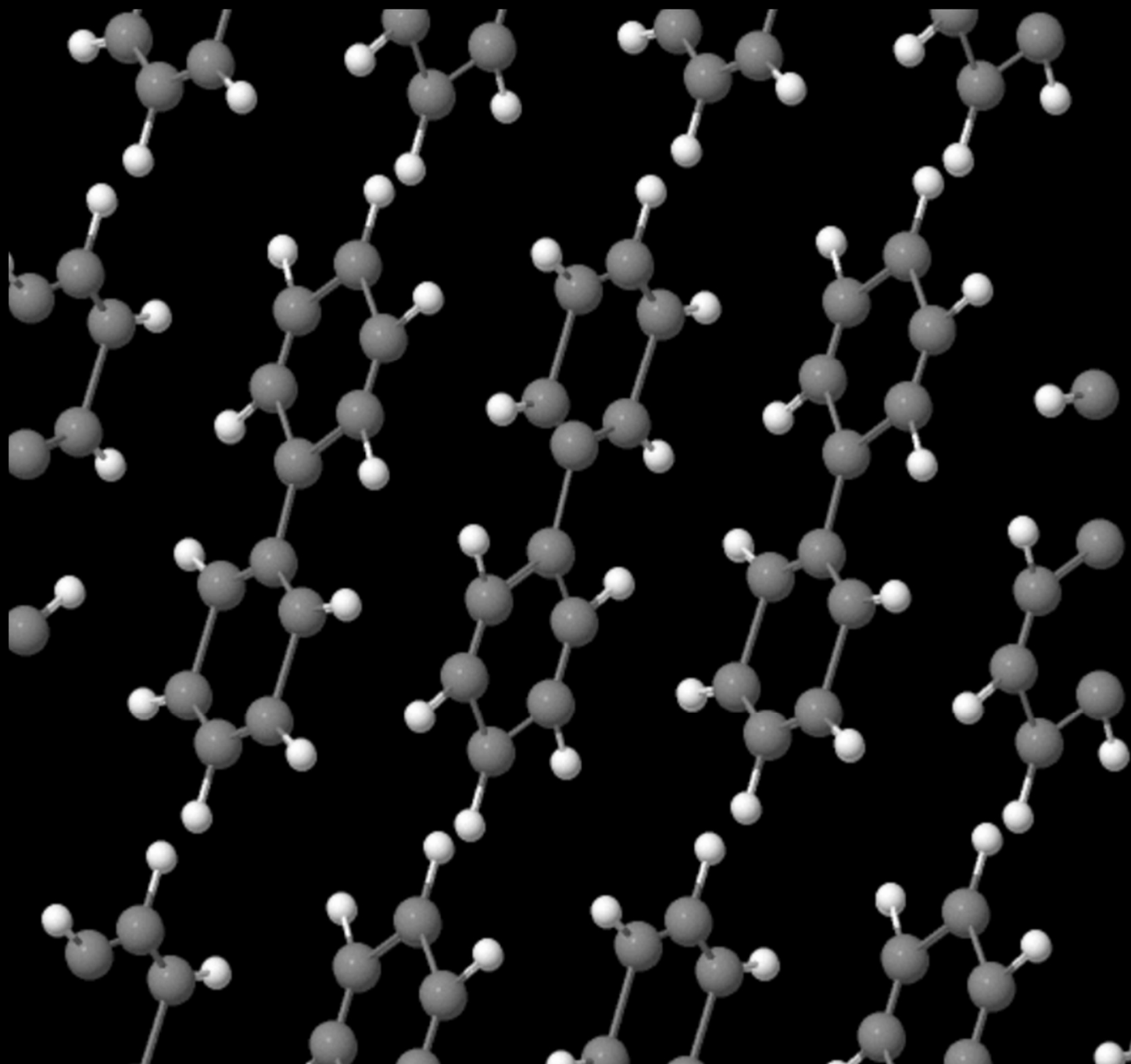


$$\omega^2 = C \left(\frac{1}{M_1} + \frac{1}{M_2} \right) \pm C \sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4 \sin^2 ka}{M_1 M_2}}$$

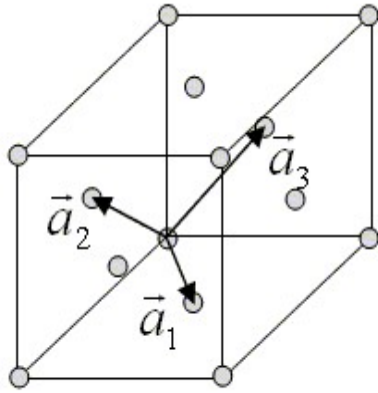
Linear chain M_1 and M_2



The branches of the dispersion curves can be translated by a reciprocal lattice vector \vec{G} .



fcc



$$\vec{a}_1 = \frac{a}{2} \hat{x} + \frac{a}{2} \hat{y}$$

$$\vec{a}_2 = \frac{a}{2} \hat{x} + \frac{a}{2} \hat{z}$$

$$\vec{a}_3 = \frac{a}{2} \hat{y} + \frac{a}{2} \hat{z}$$

$$\vec{b}_1 = \frac{2\pi}{a} (\hat{k}_x + \hat{k}_y - \hat{k}_z)$$

$$\vec{b}_2 = \frac{2\pi}{a} (\hat{k}_x - \hat{k}_y + \hat{k}_z)$$

$$\vec{b}_3 = \frac{2\pi}{a} (-\hat{k}_x + \hat{k}_y + \hat{k}_z)$$

$$\begin{aligned} m \frac{d^2 u_{lmn}^x}{dt^2} = & \frac{C}{2} \left[(u_{l+1mn}^x - u_{lmn}^x) + (u_{l-1mn}^x - u_{lmn}^x) + (u_{lm+1n}^x - u_{lmn}^x) + (u_{lm-1n}^x - u_{lmn}^x) \right. \\ & + (u_{l+1mn-1}^x - u_{lmn}^x) + (u_{l-1mn+1}^x - u_{lmn}^x) + (u_{lm+1n-1}^x - u_{lmn}^x) + (u_{lm-1n+1}^x - u_{lmn}^x) \\ & + (u_{l+1mn}^y - u_{lmn}^y) + (u_{l-1mn}^y - u_{lmn}^y) - (u_{lm+1n-1}^y - u_{lmn}^y) - (u_{lm-1n+1}^y - u_{lmn}^y) \\ & \left. + (u_{lm+1n}^z - u_{lmn}^z) + (u_{lm-1n}^z - u_{lmn}^z) - (u_{l+1mn-1}^z - u_{lmn}^z) - (u_{l-1mn+1}^z - u_{lmn}^z) \right] \end{aligned}$$

and similar expressions for the y and z motion

Normal modes are eigenfunctions of T

$$u_{lmn}^x = u_{\vec{k}}^x \exp\left(i\left(l\vec{k} \cdot \vec{a}_1 + m\vec{k} \cdot \vec{a}_2 + n\vec{k} \cdot \vec{a}_3 - \omega t\right)\right)$$

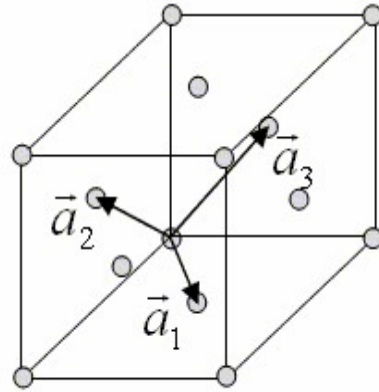
$$u_{lmn}^y = u_{\vec{k}}^y \exp\left(i\left(l\vec{k} \cdot \vec{a}_1 + m\vec{k} \cdot \vec{a}_2 + n\vec{k} \cdot \vec{a}_3 - \omega t\right)\right)$$

$$u_{lmn}^z = u_{\vec{k}}^z \exp\left(i\left(l\vec{k} \cdot \vec{a}_1 + m\vec{k} \cdot \vec{a}_2 + n\vec{k} \cdot \vec{a}_3 - \omega t\right)\right)$$

These are eigenfunctions of T.

$$\begin{aligned} T_{pqr} u_{lmn}^x &= u_{\vec{k}}^x \exp\left(i\left(l\vec{k} \cdot (\vec{a}_1 + p\vec{a}_1) + m\vec{k} \cdot (\vec{a}_2 + q\vec{a}_2) + n\vec{k} \cdot (\vec{a}_3 + r\vec{a}_3) - \omega t\right)\right) \\ &= \exp\left(i\left(lp\vec{k} \cdot \vec{a}_1 + qm\vec{k} \cdot \vec{a}_2 + rn\vec{k} \cdot \vec{a}_3\right)\right) u_{\vec{k}}^x \exp\left(i\left(l\vec{k} \cdot \vec{a}_1 + m\vec{k} \cdot \vec{a}_2 + n\vec{k} \cdot \vec{a}_3 - \omega t\right)\right) \\ &= \exp\left(i\left(lp\vec{k} \cdot \vec{a}_1 + qm\vec{k} \cdot \vec{a}_2 + rn\vec{k} \cdot \vec{a}_3\right)\right) u_{lmn}^x \end{aligned}$$

fcc



$$\vec{a}_1 = \frac{a}{2} \hat{x} + \frac{a}{2} \hat{y}$$

$$\vec{a}_2 = \frac{a}{2} \hat{x} + \frac{a}{2} \hat{z}$$

$$\vec{a}_3 = \frac{a}{2} \hat{y} + \frac{a}{2} \hat{z}$$

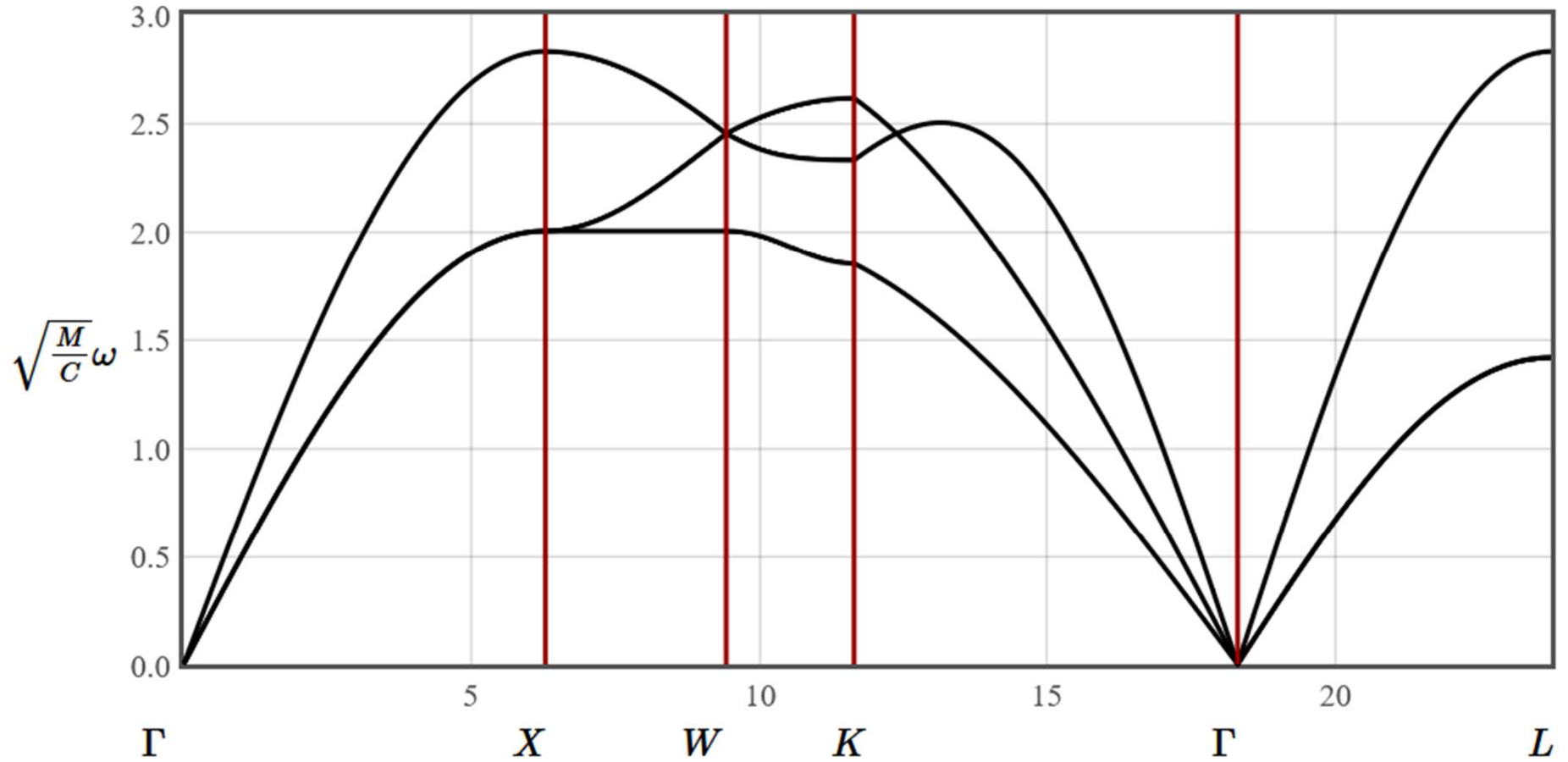
Substitute the eigenfunctions of T into Newton's laws.

$$u_{lmn}^x = u_k^x \exp\left(i\left(l\vec{k} \cdot \vec{a}_1 + m\vec{k} \cdot \vec{a}_2 + n\vec{k} \cdot \vec{a}_3\right)\right) = u_k^x \exp\left(i\left(\frac{(l+m)k_x a}{2} + \frac{(l+n)k_y a}{2} + \frac{(m+n)k_z a}{2}\right)\right).$$

$$\begin{vmatrix} 4 - \cos\left(\frac{k_x a}{2} + \frac{k_y a}{2}\right) - \cos\left(\frac{k_x a}{2} + \frac{k_z a}{2}\right) - \cos\left(\frac{k_x a}{2} - \frac{k_y a}{2}\right) - \cos\left(\frac{k_x a}{2} - \frac{k_z a}{2}\right) - \frac{m\omega^2}{\sqrt{2}C} & -\cos\left(\frac{k_x a}{2} + \frac{k_y a}{2}\right) + \cos\left(\frac{k_x a}{2} - \frac{k_y a}{2}\right) & -\cos\left(\frac{k_x a}{2} + \frac{k_z a}{2}\right) + \cos\left(\frac{k_x a}{2} - \frac{k_z a}{2}\right) \\ -\cos\left(\frac{k_x a}{2} + \frac{k_y a}{2}\right) + \cos\left(\frac{k_x a}{2} - \frac{k_y a}{2}\right) & 4 - \cos\left(\frac{k_y a}{2} + \frac{k_x a}{2}\right) - \cos\left(\frac{k_y a}{2} + \frac{k_z a}{2}\right) - \cos\left(\frac{k_y a}{2} - \frac{k_x a}{2}\right) - \cos\left(\frac{k_y a}{2} - \frac{k_z a}{2}\right) - \frac{m\omega^2}{\sqrt{2}C} & -\cos\left(\frac{k_y a}{2} + \frac{k_z a}{2}\right) + \cos\left(\frac{k_y a}{2} - \frac{k_z a}{2}\right) \\ -\cos\left(\frac{k_x a}{2} + \frac{k_z a}{2}\right) + \cos\left(\frac{k_x a}{2} - \frac{k_z a}{2}\right) & -\cos\left(\frac{k_y a}{2} + \frac{k_x a}{2}\right) + \cos\left(\frac{k_y a}{2} - \frac{k_x a}{2}\right) & 4 - \cos\left(\frac{k_z a}{2} + \frac{k_x a}{2}\right) - \cos\left(\frac{k_z a}{2} + \frac{k_y a}{2}\right) - \cos\left(\frac{k_z a}{2} - \frac{k_x a}{2}\right) - \cos\left(\frac{k_z a}{2} - \frac{k_y a}{2}\right) - \frac{m\omega^2}{\sqrt{2}C} \end{vmatrix} = 0$$

<http://lamp.tu-graz.ac.at/~hadley/ss1/phonons/fcc/fcc.html>

For every k there are 3 solutions for ω .



Phonon dispersion Au

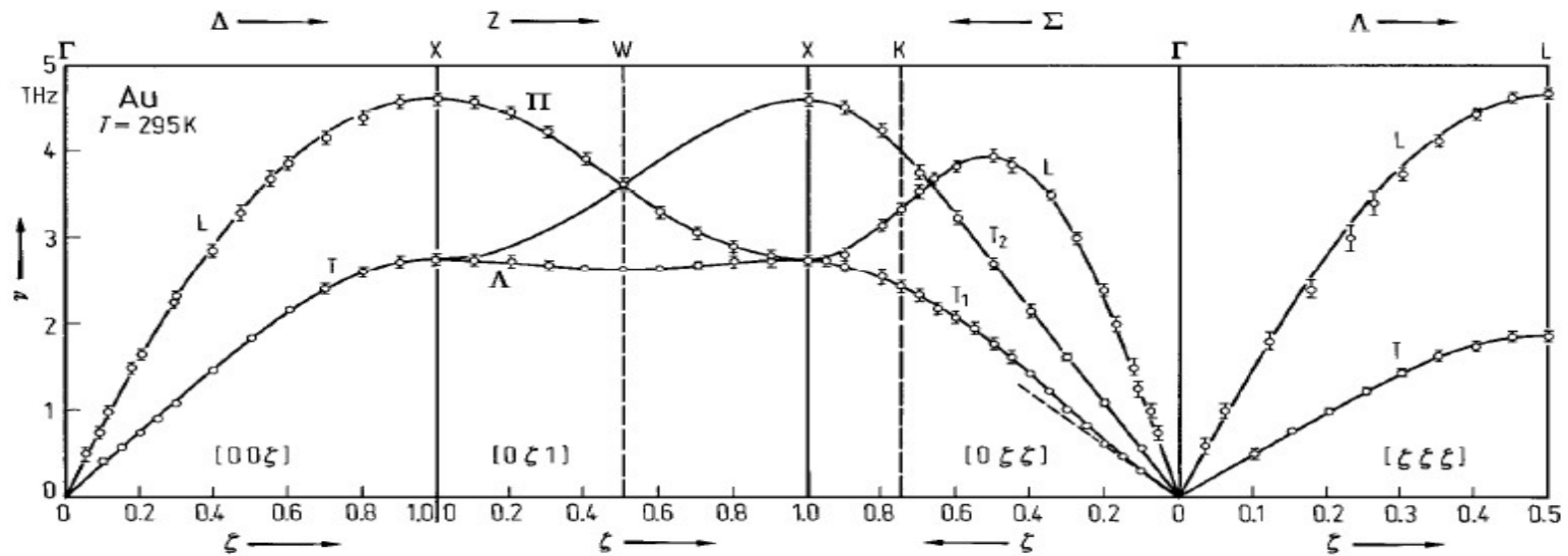
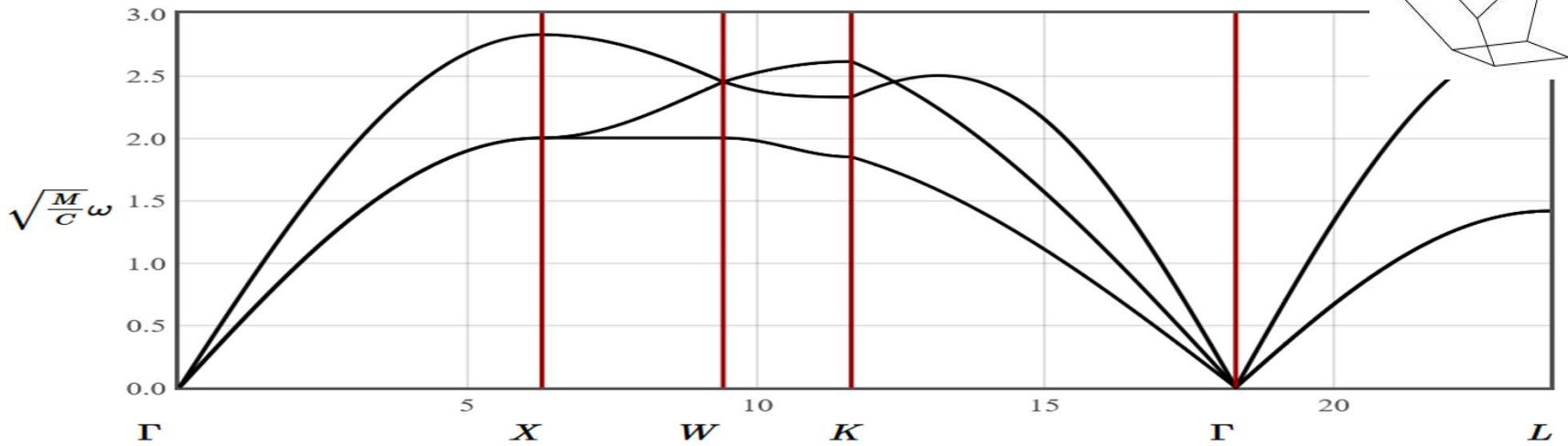
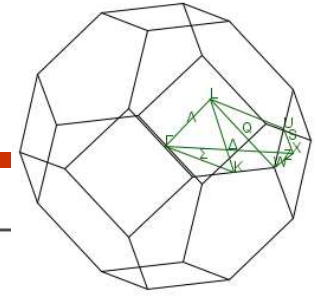
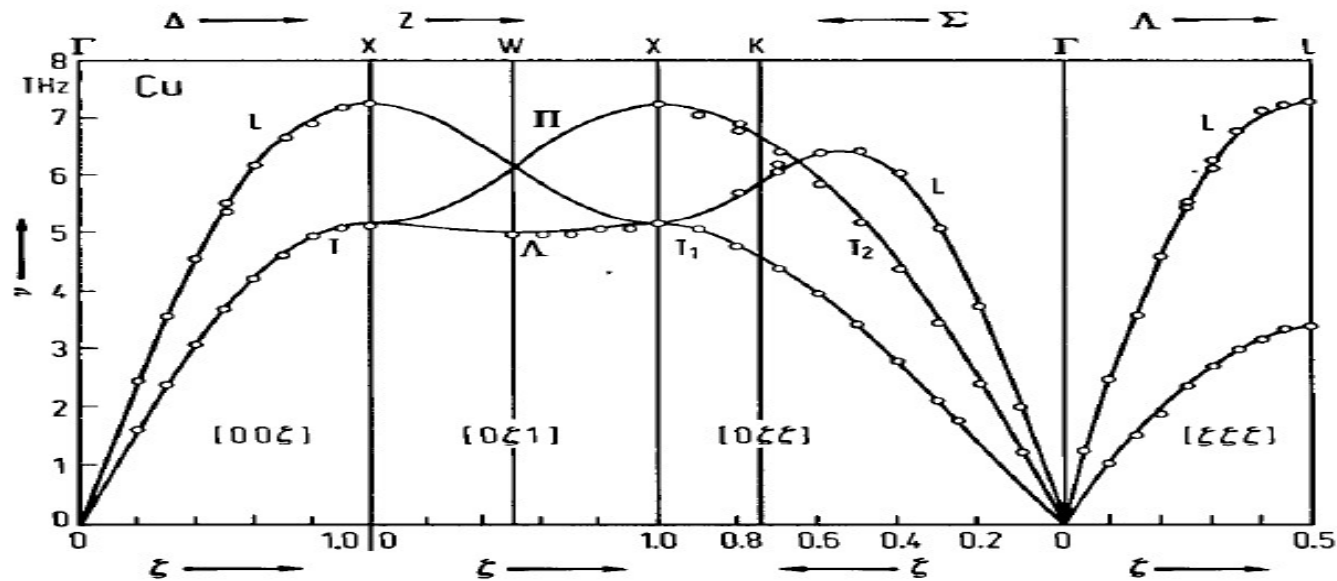
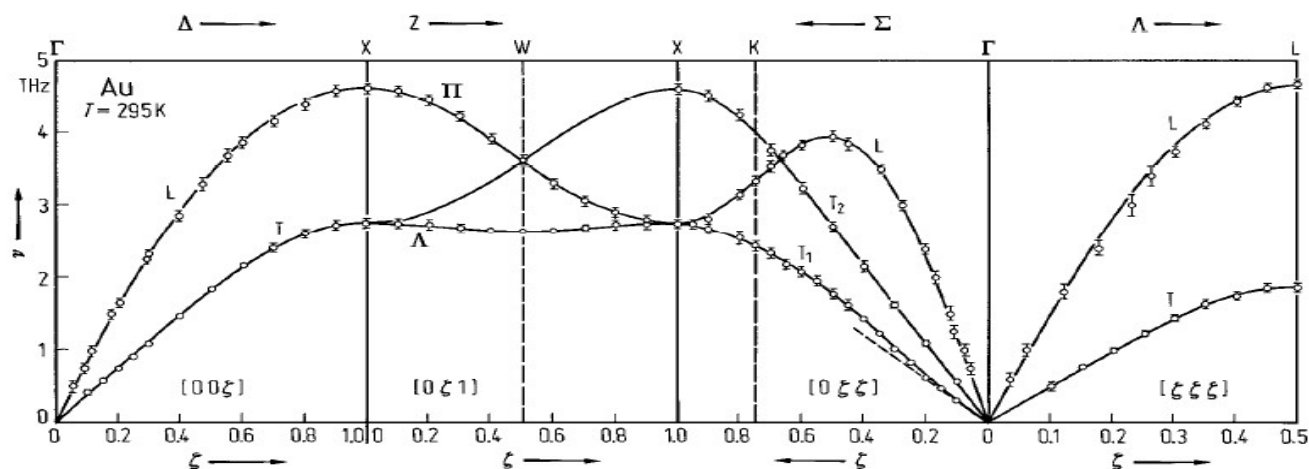


Fig. 1. Au. Phonon dispersion relations in the principal symmetry directions according to [73Ly1]. The solid curves represent both the fourth neighbour general force model (M1) and the fifth neighbour axially symmetric model (M2) of Table 3 Au. The dotted line in the Σ direction is corresponding to the velocity of sound appropriate to the $[0\zeta\zeta] T_1$ branch.

Materials with the same crystal structure will have similar phonon dispersion relations



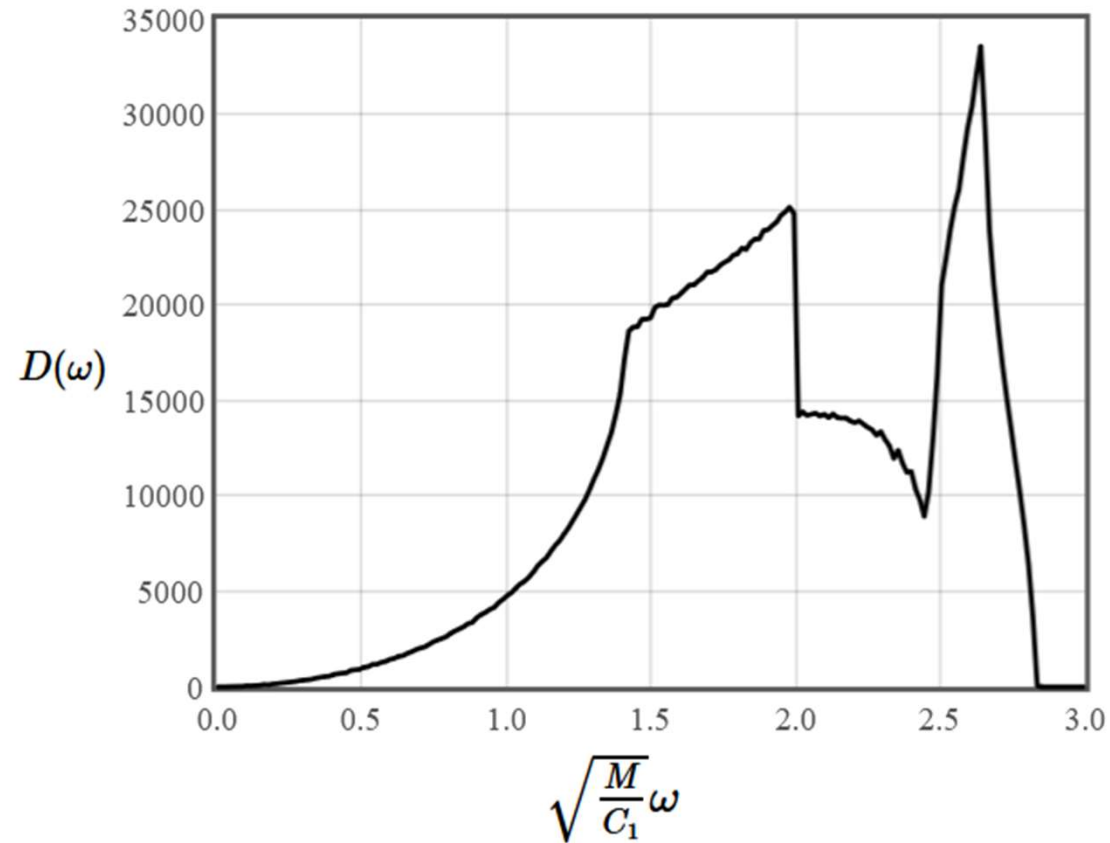
Cu



Au

Fig. 1. Au. Phonon dispersion relations in the principal symmetry directions according to [73Ly1]. The solid curves represent both the fourth neighbour general force model (M1) and the fifth neighbour axially symmetric model (M2) of Table 3 Au. The dotted line in the Σ direction is corresponding to the velocity of sound appropriate to the $[0\zeta\zeta]$ T₁ branch.

Phonon density of states of a fcc crystal



http://lampx.tugraz.at/~hadley/ss1/phonons/fcc/fcc_dos.php

Phonon DOS fcc

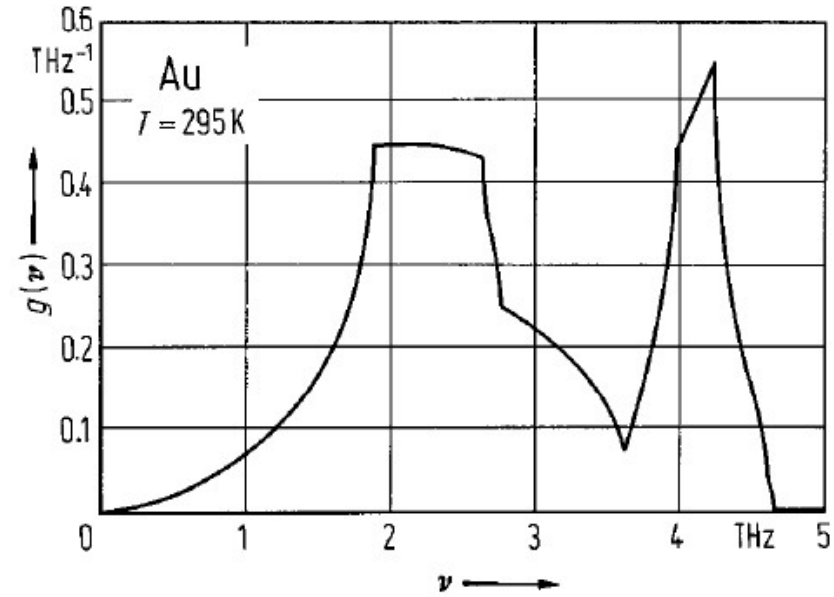
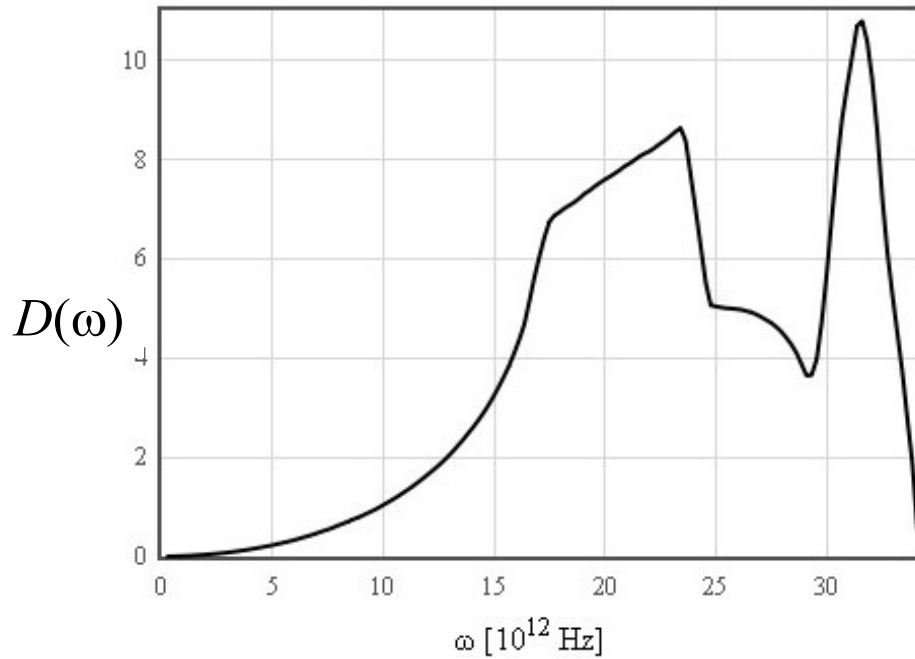
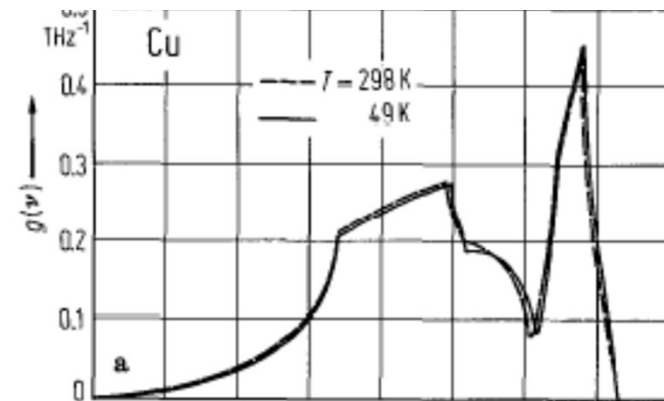
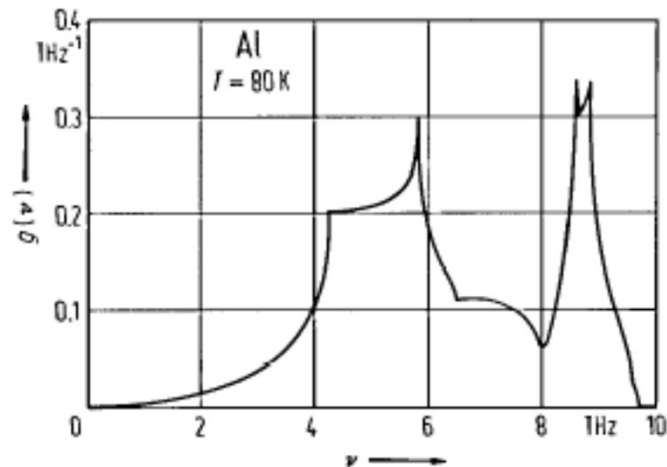
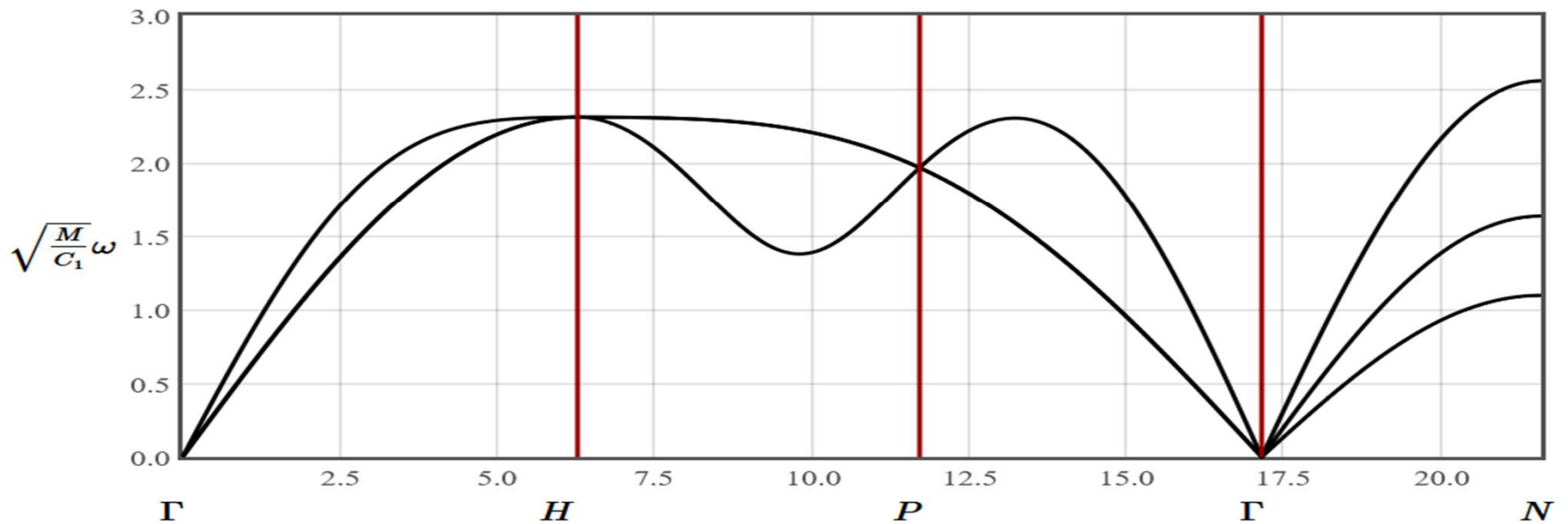
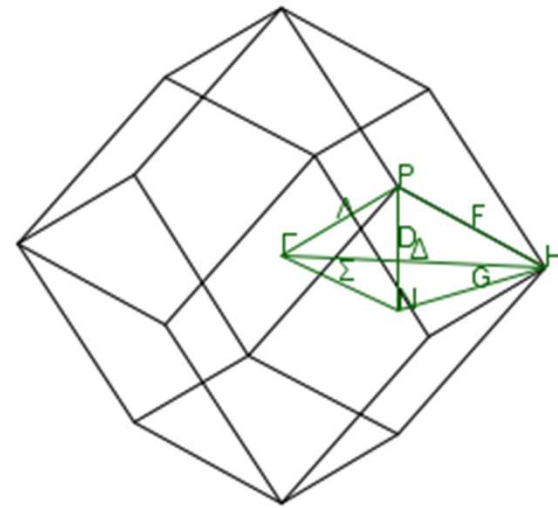
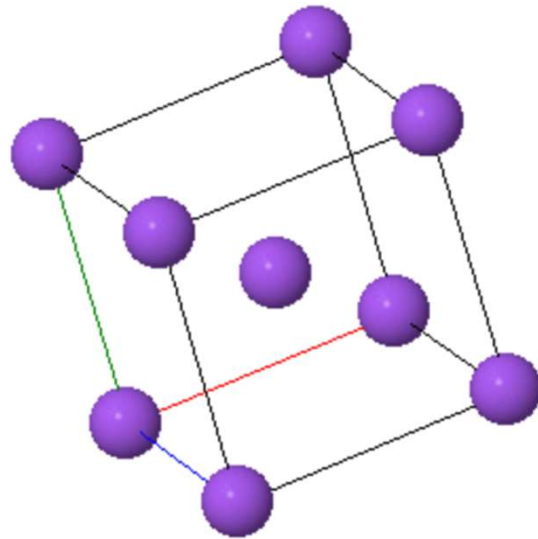


Fig. 2. Au. Frequency distribution calculated from the fourth neighbour general force constant model (M1) of Table 3 Au.



Phonon dispersion bcc



Phonon dispersion Fe

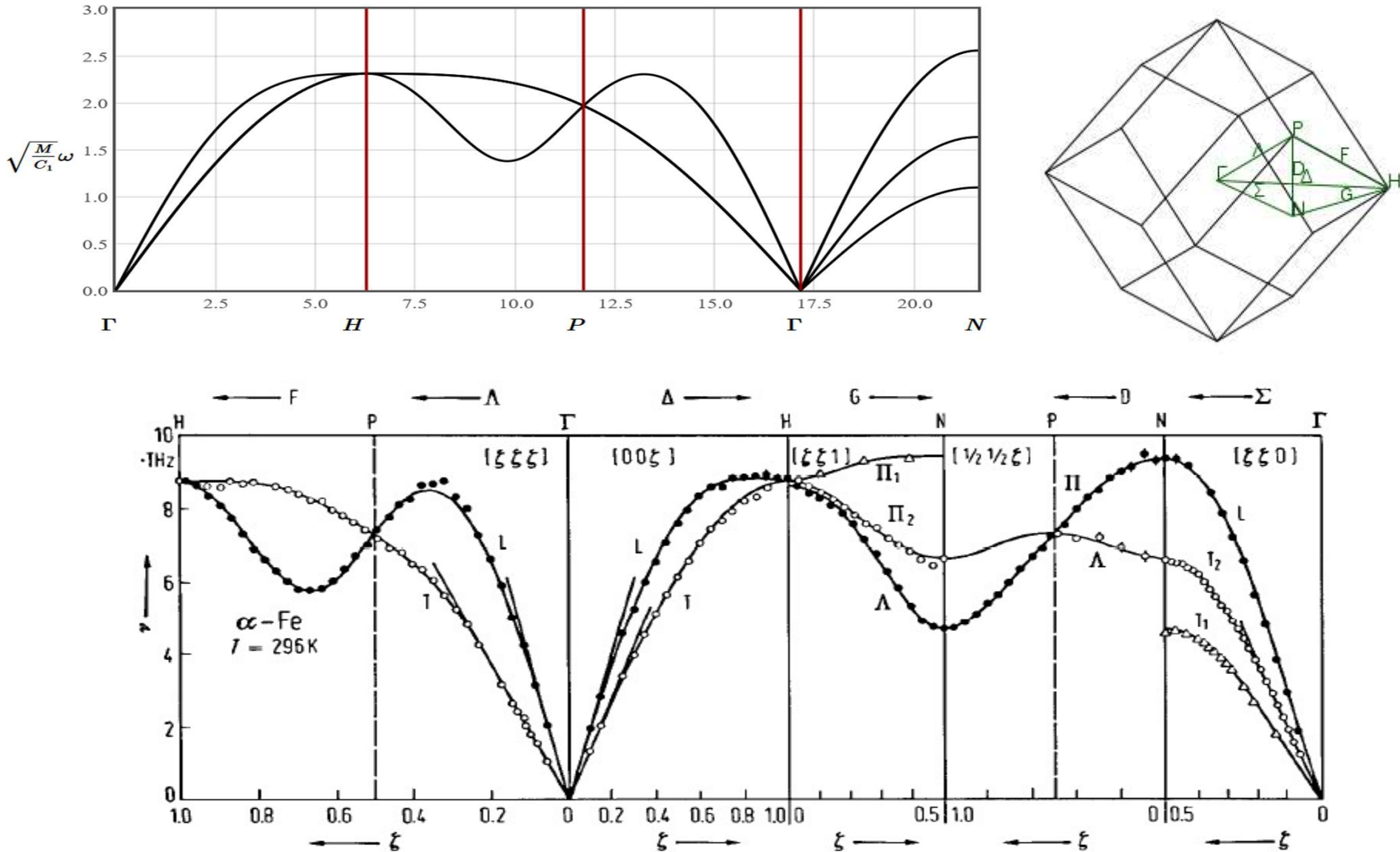


Fig. 2. Fe. Phonon dispersion curves in α -iron at 296 K. Experimental points: [68Va2]. Solid curve: fifth neighbour Born-von Karman model (Table 3 Fe [68Va2]).

From Springer Materials: Landholt Boernstein Database

Phonon DOS Fe

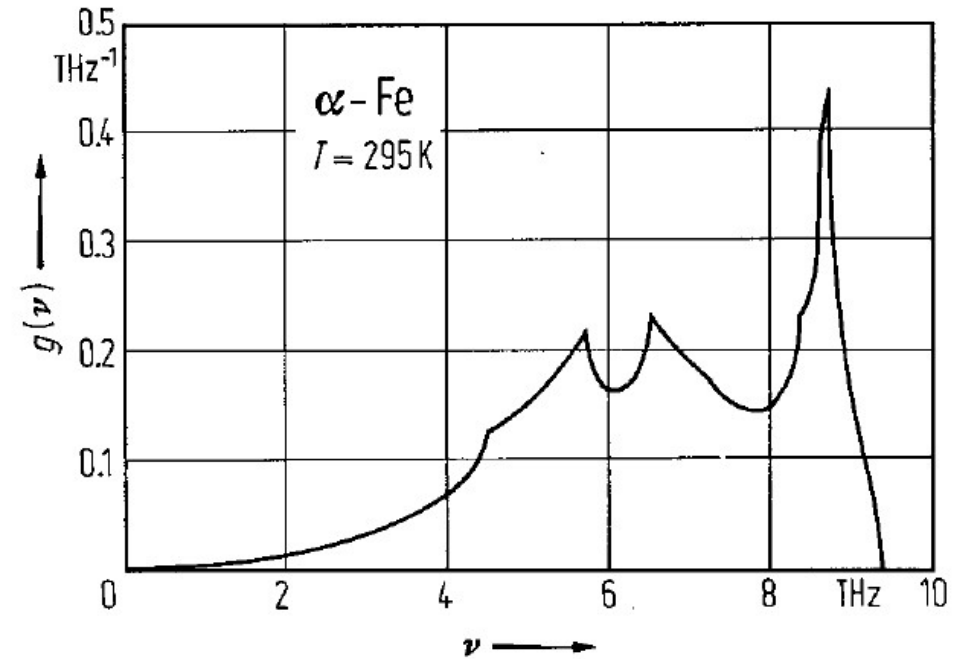
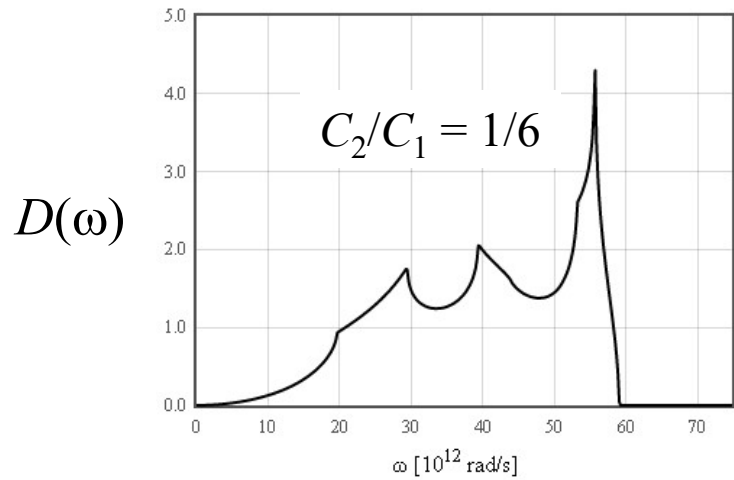
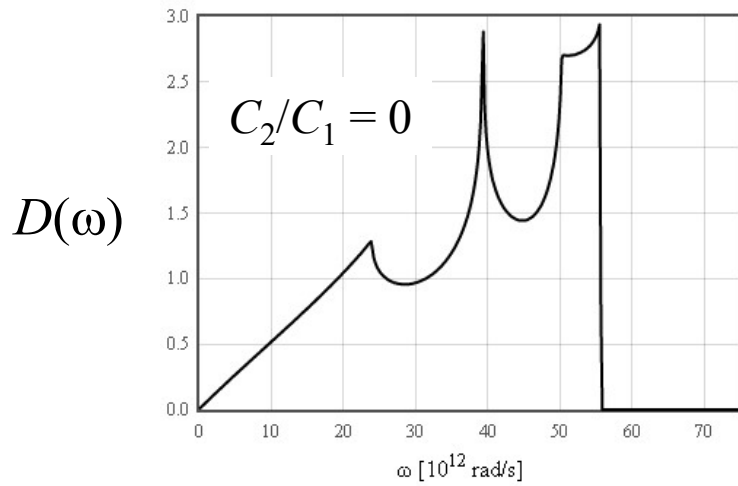
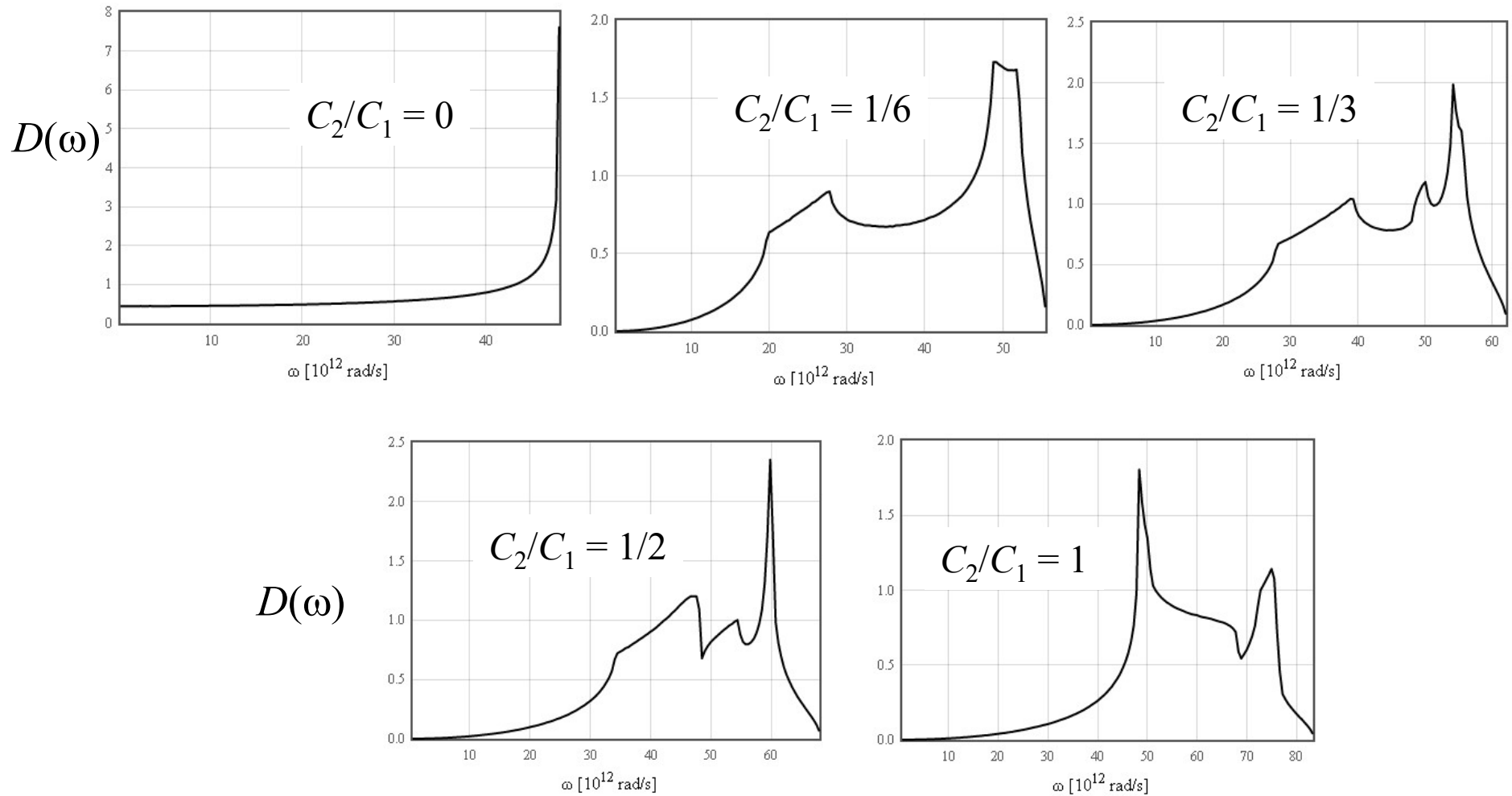


Fig. 3. Fe. Frequency spectrum of α -iron at 295 K calculated from the Born-von Karman force constants of Table 3 Fe [67Mi1].

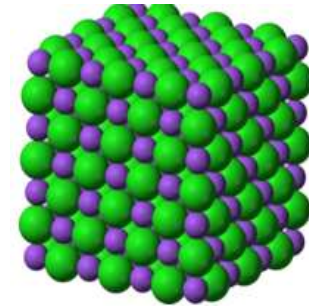
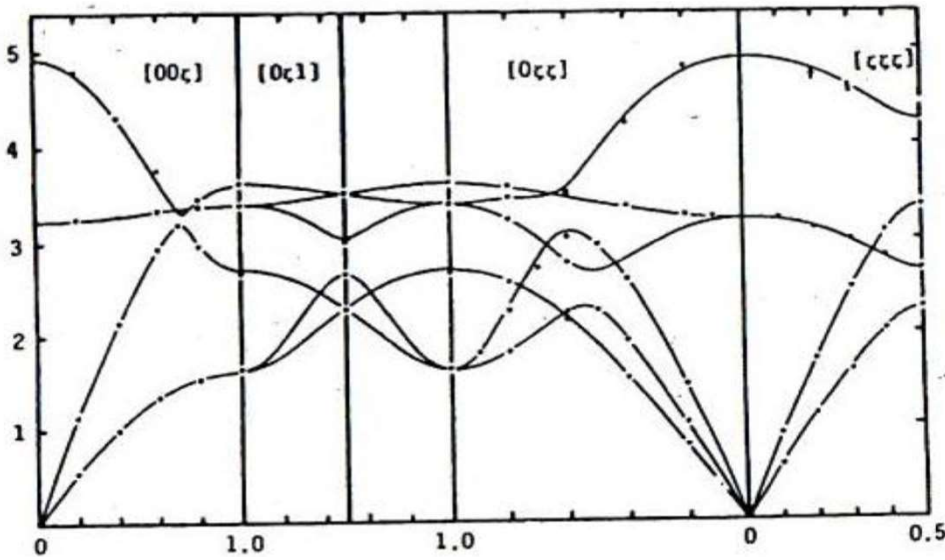
From Springer Materials: Landholt Boernstein Database

Next nearest neighbors (simple cubic)

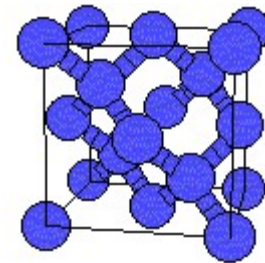
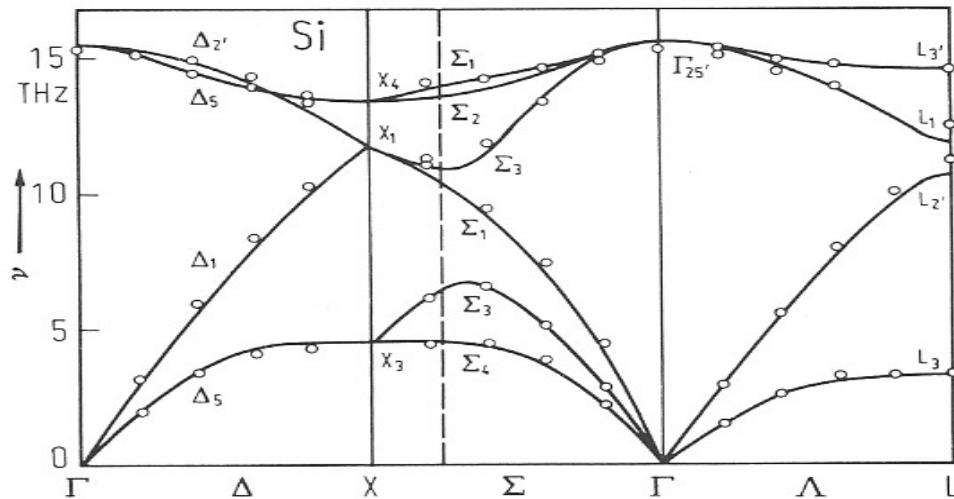


Sometimes the 5th neighbors are included.

Two atoms per primitive unit cell

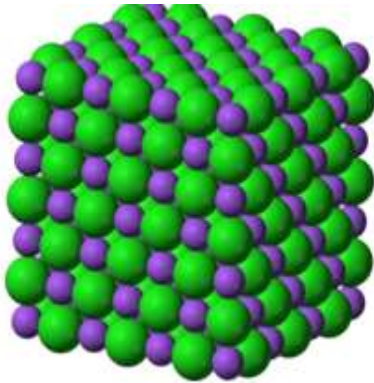


NaCl



Si

NaCl



2 atoms/unit cell

6 equations

3 acoustic and
3 optical branches

x - Richtung:

$$M_1 \frac{d^2 u_{nml}^x}{dt^2} = C \left(-2u_{nml}^x + v_{(n-1)m(l-1)}^x + v_{n(m-1)l}^x \right)$$

$$M_2 \frac{d^2 v_{nml}^x}{dt^2} = C \left(-2v_{nml}^x + u_{(n+1)m(l+1)}^x + u_{n(m+1)l}^x \right)$$

y - Richtung:

$$M_1 \frac{d^2 u_{nml}^y}{dt^2} = C \left(-2u_{nml}^y + v_{(n-1)(m-1)l}^y + v_{nm(l-1)}^y \right)$$

$$M_2 \frac{d^2 v_{nml}^y}{dt^2} = C \left(-2v_{nml}^y + u_{(n+1)(m+1)l}^y + u_{nm(l+1)}^y \right)$$

z - Richtung:

$$M_1 \frac{d^2 u_{nml}^z}{dt^2} = C \left(-2u_{nml}^z + v_{n(m-1)(l-1)}^z + v_{(n-1)ml}^z \right)$$

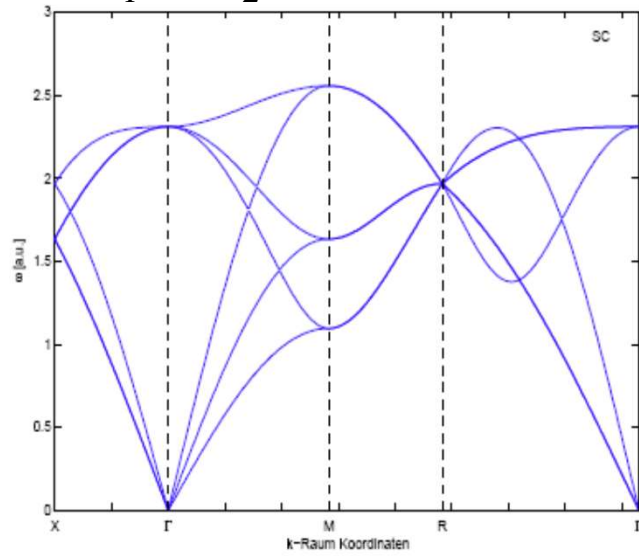
$$M_2 \frac{d^2 v_{nml}^z}{dt^2} = C \left(-2v_{nml}^z + u_{n(m+1)(l+1)}^z + u_{(n+1)ml}^z \right)$$

$$u_{nml}^x = u_{\vec{k}}^x \exp\left(i\left(\vec{k} \cdot \vec{a}_1 + \vec{k} \cdot \vec{a}_2 + \vec{k} \cdot \vec{a}_3 - \omega t\right)\right) \quad v_{nml}^x = v_{\vec{k}}^x \exp\left(i\left(\vec{k} \cdot \vec{a}_1 + \vec{k} \cdot \vec{a}_2 + \vec{k} \cdot \vec{a}_3 - \omega t\right)\right)$$

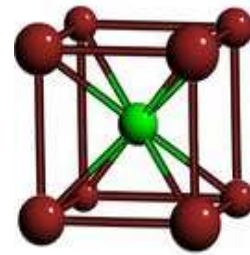
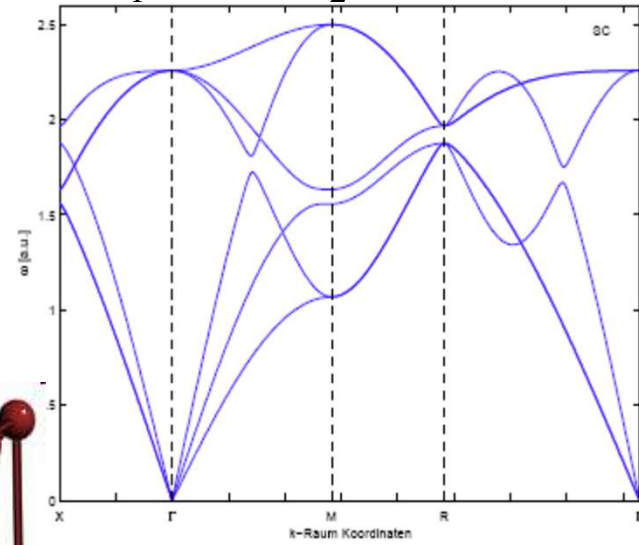
CsCl

Hannes Brandner

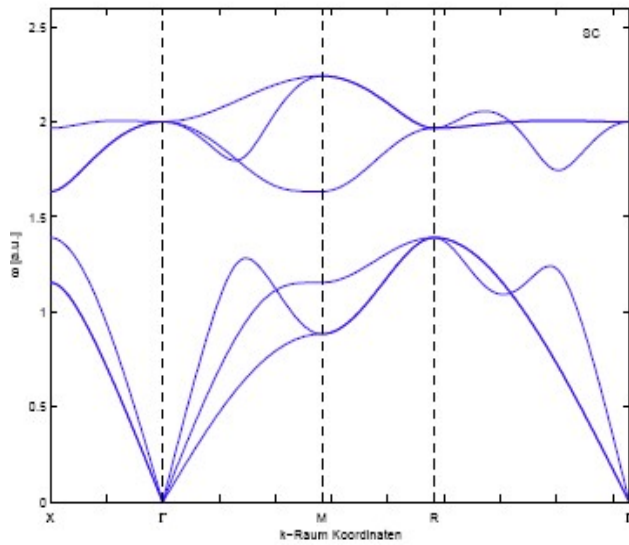
$$M_1 = M_2$$



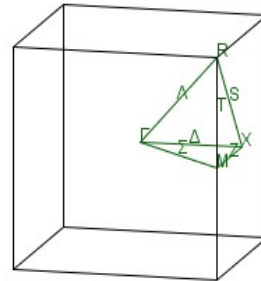
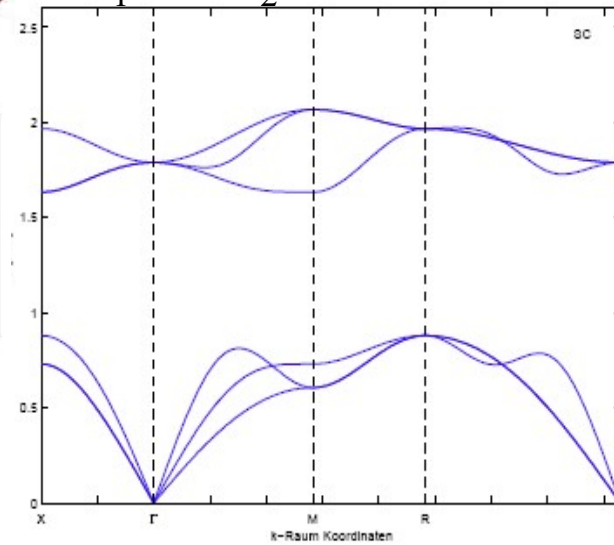
$$M_1 = 1.1 M_2$$



$$M_1 = 2M_2$$



$$M_1 = 5M_2$$



3 dimensions

N atoms

$3N$ normal modes

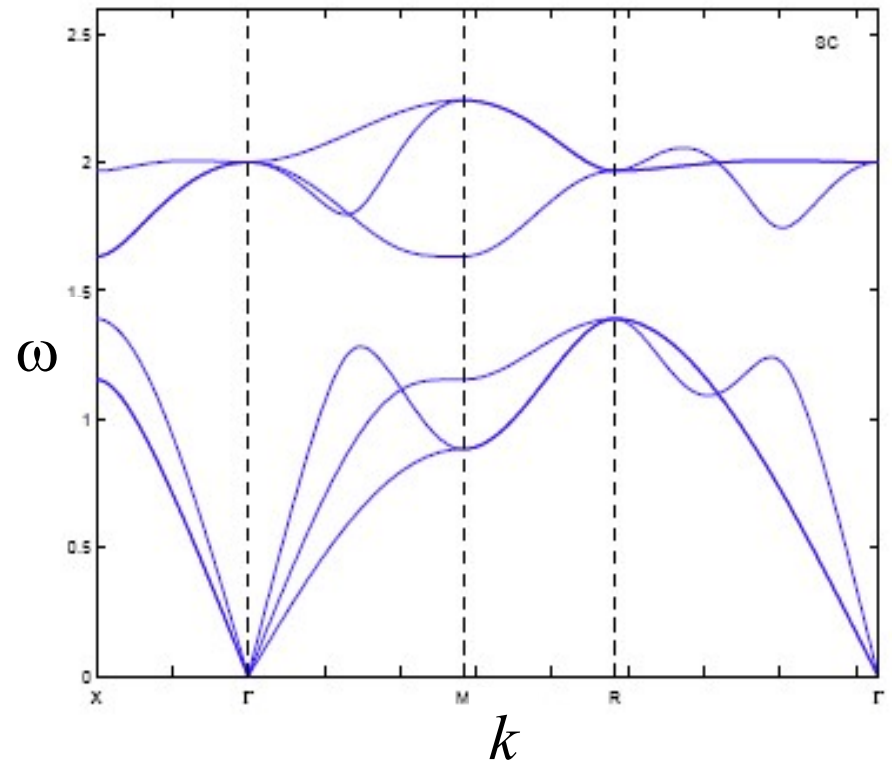
p atoms per unit cell

N/p unit cells = k vectors

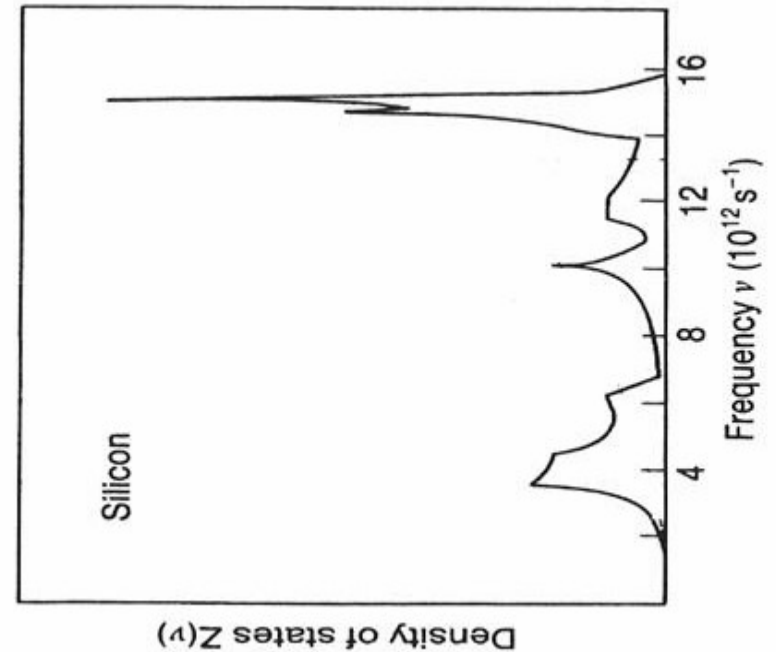
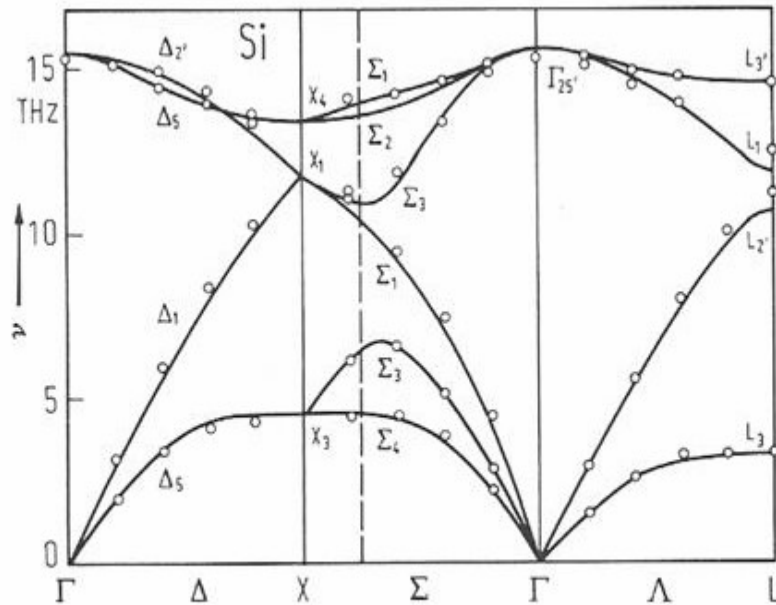
$3p$ branches to the dispersion relation

3 acoustic modes (1 longitudinal, 2 transverse)

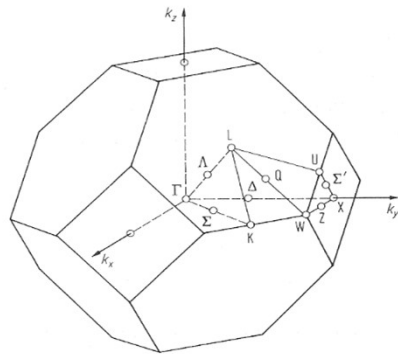
$3p - 3$ optical modes



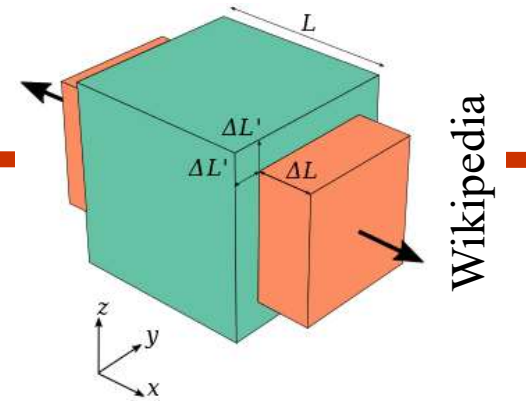
Silicon phonon dispersion, DOS



Different speeds of sound for different directions and polarizations causes dispersion of pulses.



Poisson's ratio



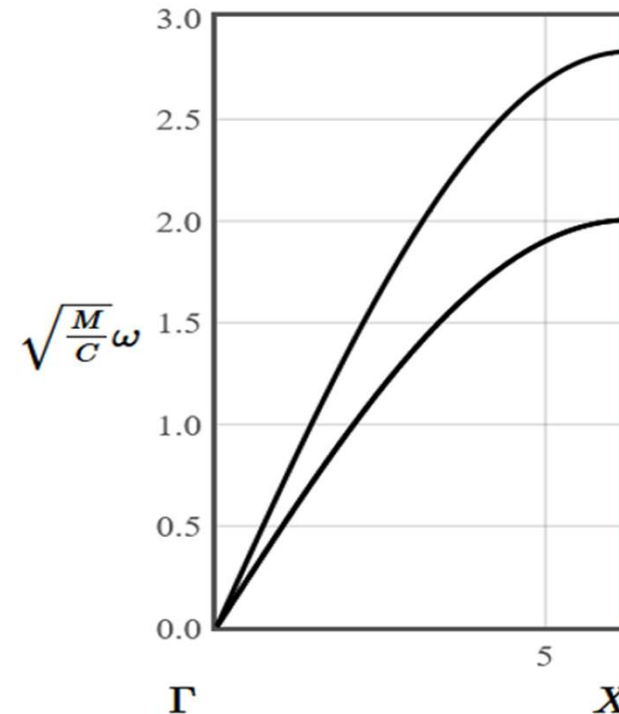
E - Elastic constant

ν - Poisson's ratio

ρ - density

$$c_T = \sqrt{\frac{E(1-\nu)}{\rho(1-\nu-2\nu^2)}}$$

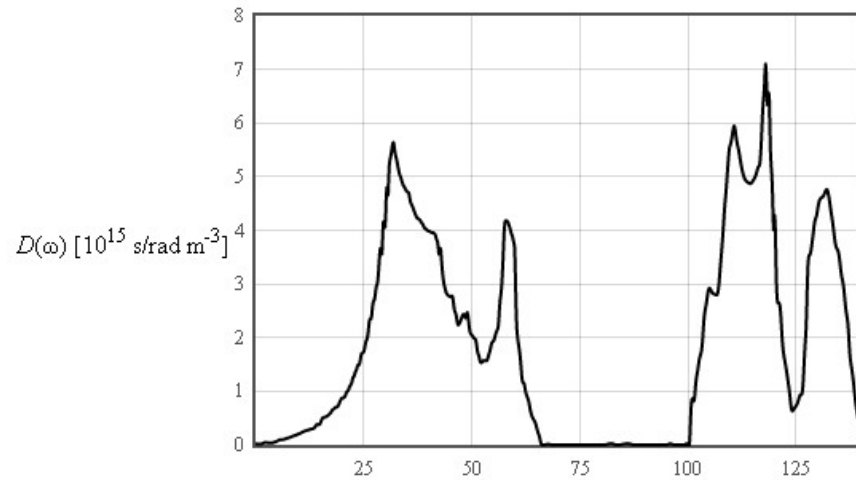
$$c_L = \sqrt{\frac{E}{2\rho(1+\nu)}}$$



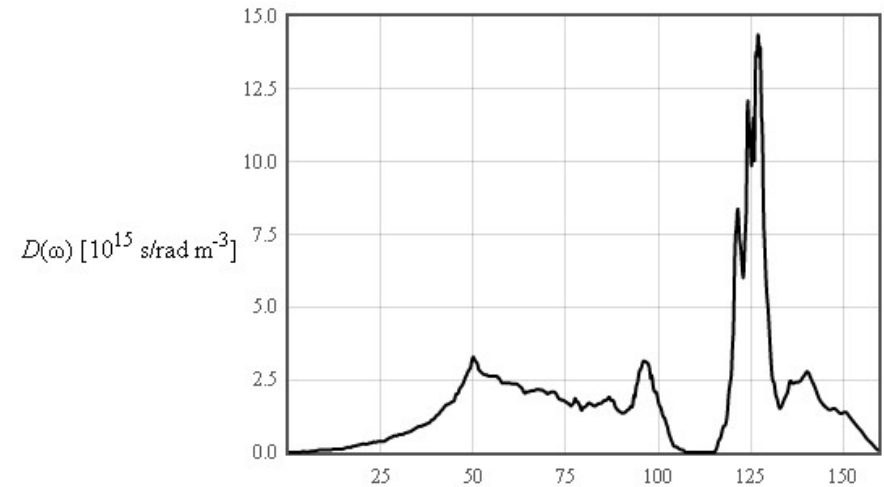
If the density is known, you can determine E and ν .

Two atoms per primitive unit cell

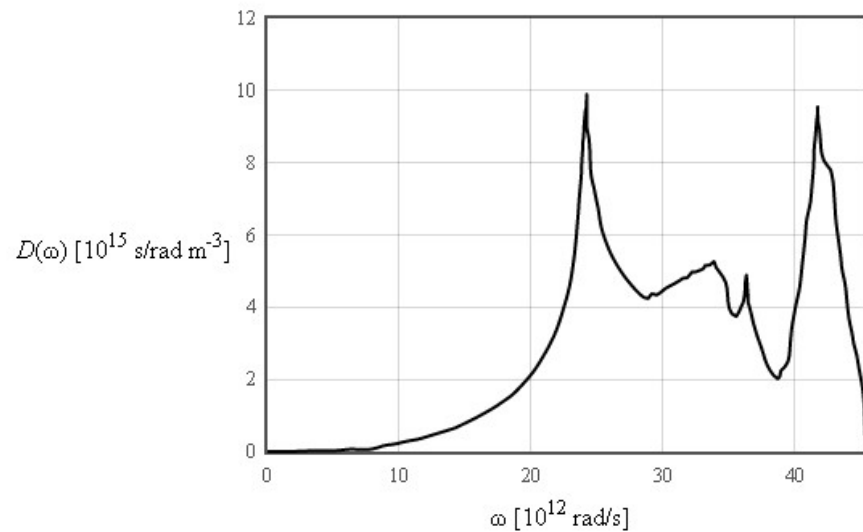
Phonon density of states for GaN



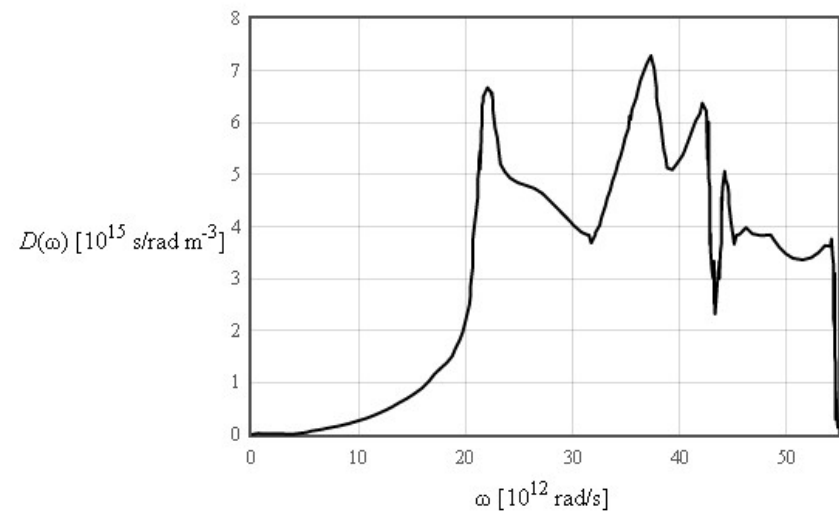
Phonon density of states for AlN

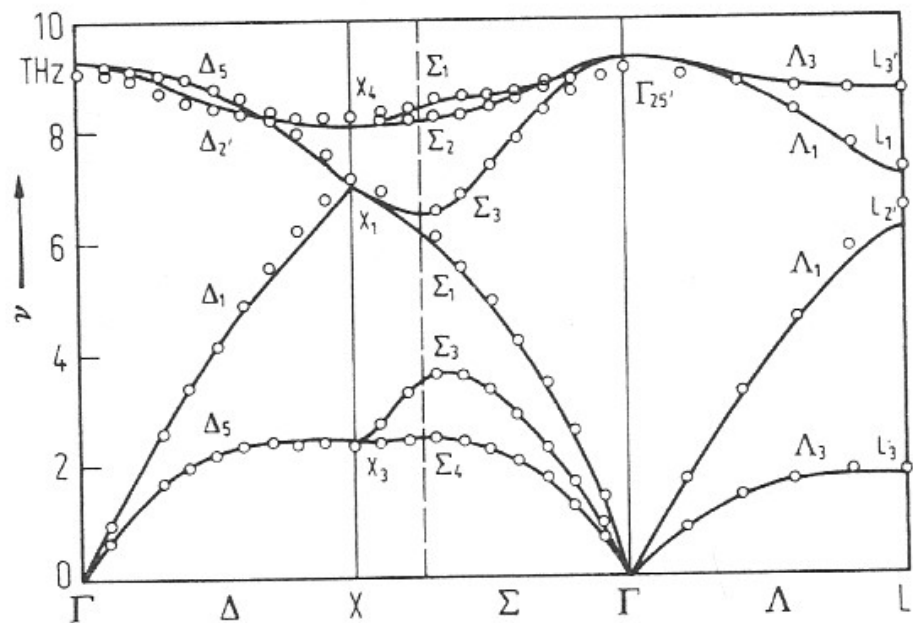
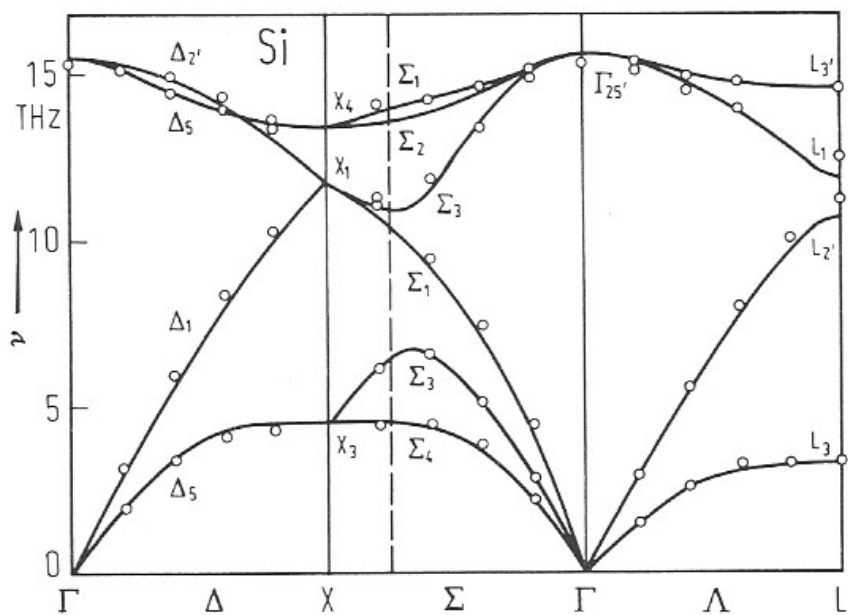


Phonon density of states for hcp magnesium



Phonon density of states for hcp titanium





Ge, C, α -Sn ?

